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Multispherical Euclidean distance matrices

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ABSTRACT

In this paper we introduce new necessary and sufficient conditions for an Euclidean distance matrix to be multispherical. The class of multispherical distance matrices studied in this paper contains not only most of the matrices studied by Hayden et al. (1996) [2], but also many other multispherical structures that do not satisfy the conditions in Hayden et al. (1996) [2].

We also study the information provided by the origin of coordinates when it is placed at the center of the spheres and the origin representation property is satisfied. These vectors associated with the origin of coordinates generate a number of supporting hyperplanes for a family of multispherical matrices and also describe part of the null space of the corresponding distance matrices.

1. Introduction and preliminaries

We begin by introducing basic notation and definitions. The set of *symmetric matrices* of order n will be denoted by S_n, and by Ω_n we indicate the set of *symmetric positive semidefinite matrices*. It is important to recall that Ω_n is a closed convex cone. A linear subspace generated by the vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ will be denoted by $span\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$. The vector with all ones is denoted by $\mathbf{e}$, and M is the orthogonal complement of $span\{\mathbf{e}\}$ in $\Re^n$.

A *predistance matrix* is a symmetric and nonnegative matrix with zero diagonal entries. An $n \times n$ predistance matrix $D = (d_{ij})$ is called a *Euclidean Distance Matrix* (EDM), if there exist n points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \Re^r$ for some r such that

$$d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2 .$$

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Observe that the entries of D are squared inter-point distances. We say that a distance matrix D is *spherical* if the points generating D lie on the surface of a sphere. If the points lie on $k(< n)$ spheres each centered at the origin, then the EDM is said to be *multispherical*.

Let Λ_n be the set of all EDMs of order n, which forms a convex cone. As shown in Gower [1] and Johnson and Tarazaga [3], the set Λ_n is the image under a linear function defined on the cone Ω_n. More precisely, by defining the linear function

$$\kappa(B) = \mathbf{b}\mathbf{e}^t + \mathbf{e}\mathbf{b}^t - 2B, \quad B \in \Omega_n,$$

where $\mathbf{b}$ is the vector consisting of the diagonal entries of B, we have $\kappa(\Omega_n) = \Lambda_n$. Let $\mathbf{s}$ be an $n \times 1$ vector. A maximal face of the set Ω_n is defined by

$$\Omega_n(\mathbf{s}) = \{X \in \Omega_n | X\mathbf{s} = 0\}.$$

Let us consider maximal faces $\Omega_n(\mathbf{s})$ with $\mathbf{s}$ satisfying $\mathbf{s}^t\mathbf{e} \neq 0$. When κ is restricted to such maximal faces, it becomes one-to-one, and the inverse function is given by

$$\tau_s(D) = -\frac{1}{2}\left(I - \mathbf{e}\mathbf{s}^t\right) D \left(I - \mathbf{s}\mathbf{e}^t\right).$$

Note that this is a family of right inverses for the application κ. Every face $\Omega_n(\mathbf{s})$ with $\mathbf{s}^t\mathbf{e} = 1$ corresponds to a fixed location of the origin of coordinates. Changes of faces represent translations of the origin of coordinates (for more information, see Section 2 of [3]).

If X is a coordinate matrix for D in the system of coordinates $\mathbf{s}$, then $XX^t\mathbf{s} = 0$ and $X^t\mathbf{s} = 0$ hold. Here, the condition $\mathbf{s}^t\mathbf{e} = 1$ means that the origin of coordinates is in the affine variety generated by the columns of X^t. An important case is the one in which $\mathbf{s} = \mathbf{e}/n$. In this case we will denote $\tau_{e/n}$ just by τ, and τ and κ are inverse to each other between Λ_n and $\Omega_n(\mathbf{e})$. Matrices in $\Omega_n(\mathbf{e})$ are called *centered* positive semidefinite matrices and the origin of coordinates is set at the centroid of the configuration points.

Let us denote by $\mathcal{N}$ the set of the first n natural numbers: $\mathcal{N} = \{1, 2, \ldots, n\}$, and consider a partition of $\mathcal{N}$ into $k(< n)$ nonempty subsets, which is denoted by $\mathcal{N}_i$ with cardinality n_i $(i = 1, \ldots, k)$. Note that $\sum_{i=1}^k n_i = n$. We assume without loss of generality that $\mathcal{N}_1 = \{1, \ldots, n_1\}, \mathcal{N}_2 = \{n_1 + 1, \ldots, n_1 + n_2\}$, and so on. Given a vector $\mathbf{x} \in \Re^n$, let $\mathbf{x}_{\mathcal{N}_i}$ or $\mathbf{x}_i$ denote the restriction of the vector $\mathbf{x}$ to $\mathcal{N}_i$. Given a coordinate matrix X, let $X_{\mathcal{N}_i}$ denote the submatrix of X whose row vectors have indexes in $\mathcal{N}_i$. We say that a vector $\mathbf{x}$ has block structure (or it is a blocked vector) with respect to the partition $\mathcal{N}_i$ $(i = 1, \ldots, k)$, if $\mathbf{x}_{\mathcal{N}_i}$ is a constant vector for each $i = 1, \ldots, k$.

With the above partition $\mathcal{N}_i$ $(i = 1, \ldots, k)$, let $\mathbf{s}$ be an $n \times 1$ vector such that

$$\mathbf{s}^t\mathbf{e} = n \quad \text{and} \quad \mathbf{s}_i^t\mathbf{e}_i = n_i \ (i = 1, \ldots, k), \tag{1.1}$$

where the vectors $\mathbf{s}_i \in \Re^{n_i}$ and $\mathbf{e}_i \in \Re^{n_i}$ are the restrictions of $\mathbf{s}$ and $\mathbf{e}$, respectively

$$\mathbf{s}_i = \mathbf{s}_{\mathcal{N}_i} \quad \text{and} \quad \mathbf{e}_i = \mathbf{e}_{\mathcal{N}_i}. \tag{1.2}$$

The equalities $\mathbf{s} = (\mathbf{s}_1^t, \ldots, \mathbf{s}_k^t)^t$ and $\mathbf{e} = (\mathbf{e}_1^t, \ldots, \mathbf{e}_k^t)^t$ are clear. We fix the vector $\mathbf{s}$ and the partition $\mathcal{N}_i$ $(i = 1, \ldots, k)$ throughout this paper.

By using the vectors $\mathbf{s}$, $\mathbf{s}_i$ and $\mathbf{e}_i$, we define the $n \times k$ matrices $\overline{S}$ and $\overline{E}$ by

$$\overline{S} = \begin{pmatrix} \mathbf{s}_1 & & 0 \\ & \ddots & \\ 0 & & \mathbf{s}_k \end{pmatrix} = \text{block-diag}\{\mathbf{s}_1, \ldots, \mathbf{s}_k\}, \tag{1.3}$$

$$\overline{E} = \begin{pmatrix} \mathbf{e}_1 & & 0 \\ & \ddots & \\ 0 & & \mathbf{e}_k \end{pmatrix} = \text{block-diag}\{\mathbf{e}_1, \ldots, \mathbf{e}_k\},$$

respectively. Corresponding to $\overline{S}$, we denote by S the $n \times n$ diagonal matrix whose diagonal entries are $\mathbf{s}$:

$$S = \mathrm{diag}(\mathbf{s}). \tag{1.4}$$

The following relation is easy to obtain:

$$\overline{S} = S\overline{E}. \tag{1.5}$$

As is defined in [2], for given $\mathbf{s}$ in (1.1), an $n \times n$ symmetric matrix D has $\mathbf{s}$-block structure if there exists a $k \times k$ matrix $A = (a_{ij})$ such that

$$D_{ij}\mathbf{s}_j = a_{ij}\mathbf{e}_i \quad (i, j = 1, \ldots, k), \tag{1.6}$$

where $D_{ij} : n_i \times n_j$ is the (i, j)th block of D. This condition can be restated in matrix form as

$$D\overline{S} = \overline{E}A. \tag{1.7}$$

The expression can be compared with that of a spherical EDM. As is shown in Tarazaga et al. [5], an EDM $D : n \times n$ is spherical if and only if it admits the expression

$$D\mathbf{s} = a\mathbf{e}$$

for some real number $a \in \Re$ and some $\mathbf{s} \in \Re^n$ such that $\mathbf{s}^t\mathbf{e} \neq 0$.

The following theorem was established in [2].

Theorem 1 (Theorem 4.1 of [2]). *Let D be an EDM. The followings are equivalent*:

(a) *There exists a vector* $\mathbf{x} \in \Re^n$ *such that* $\mathbf{x}^t\mathbf{e} = 1$ *and* $D\mathbf{x}$ *has block structure, that is,*

$$D\mathbf{x} = (v_1, \ldots, v_1, v_2, \ldots, v_2, \ldots, v_k, \ldots, v_k)^t,$$

the blocks having length $n_1, \ldots, n_k$*, respectively, and* $n_1 + \cdots + n_k = n$ $(k < n)$.

(b) *There exist n generating points* $\mathbf{p}_1, \ldots, \mathbf{p}_n$ *for D that lie on k spheres* $\mathbb{S}_1, \ldots, \mathbb{S}_k$ *each centered at the origin. The sphere* $\mathbb{S}_1$ *has radius* R_1 *and contains* $\mathbf{p}_1, \ldots, \mathbf{p}_{n_1}$; $\mathbb{S}_2$ *has radius* R_2 *and contains* $\mathbf{p}_{n_1+1}, \ldots, \mathbf{p}_{n_1+n_2}$, *etc.*

It is worthy to mention that this is a quite general theorem that links general multispherical configurations [the part (b) of the theorem] with the existence of system of coordinate $\mathbf{x}$ such that $D\mathbf{x}$ is a blocked vector [the part (a)]. The equality in (a) can be rewritten as

$$D\mathbf{x} = \overline{E}\mathbf{v} \quad \text{with } \mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_k \end{pmatrix} \in \Re^k.$$

An important special case of the Theorem 1 is discussed in [2], where the matrix D has $\mathbf{s}$-block structure and the associated matrix $A = (a_{ij})$ satisfies

$$\frac{a_{ij}}{n_j} = \frac{a_{ji}}{n_i} = \frac{a_{ii}}{2n_i} + \frac{a_{jj}}{2n_j} \quad (i, j = 1, \ldots, k). \tag{1.8}$$

Note that the vector $\mathbf{s}$ is assumed to be nonnegative, which is an important restriction. The result is as follows.

Theorem 2 (Theorem 4.2 of [2]). *Let D be an EDM, and suppose that* $\mathbf{s}_1, \ldots, \mathbf{s}_k$ *are nonnegative. The following are equivalent*:

(a) *There exists a* $k \times k$ *matrix* $A = (a_{ij})$ *such that* (1.6) *and* (1.8) *hold*.
(b) *There exist* n *generating points* $\mathbf{p}_1, \ldots, \mathbf{p}_n$ *for* D *that lie on* k *spheres* $\mathbb{S}_1, \ldots, \mathbb{S}_k$ *each centered at the origin. The sphere* $\mathbb{S}_1$ *contains* $\mathbf{p}_1, \ldots, \mathbf{p}_{n_1}$; $\mathbb{S}_2$ *contains* $\mathbf{p}_{n_1+1}, \ldots, \mathbf{p}_{n_1+n_2}$, *etc., and each of the separate spherical configurations has the origin in its convex hull*.
(c) *The matrix* DS *has* k *block eigenvectors that belong to the null space of* BS.

2. Conditions for block structure

Let $\mathbf{s} \in \Re^n$ and $\mathcal{N}_i$ $(i = 1, \ldots, k)$ be as in (1.1) and fix them throughout this section. In this section, we derive two conditions for an EDM D to have $\mathbf{s}$-block structure for the vector $\mathbf{s} \in \Re^n$. Recall that $\mathbf{e}_i$ is the $n_i \times 1$ vector of all ones, and let F_i be any $n_i \times (n_i - 1)$ matrix satisfying

$$F_i^t \mathbf{e}_i = 0 \quad \text{and} \quad F_i^t F_i = I.$$

Set

$$\overline{F} = \begin{pmatrix} F_1 & & \\ & \ddots & \\ & & F_k \end{pmatrix} = \text{block-diag}\{F_1, \ldots, F_k\} : n \times (n-k). \tag{2.1}$$

Clearly, the matrix F satisfies

$$\overline{F}^t \overline{E} = 0 \quad \text{and} \quad \text{rank}\overline{F} = n - k, \tag{2.2}$$

which shows that the linear subspace spanned by the column vectors of $\overline{F}$ is the orthogonal complement of the subspace spanned by the column vectors of $\overline{E}$.

The following matrix result is well known in the context of linear statistical inference. For detail, see, for example, Theorem 8.2.1 and Corollary 3 of Rao and Mitra [4].

Lemma 1. *Let* H *be an* $n \times n$ *positive semidefinite matrix, and let* Y *be an* $n \times k$ *matrix of rank* k. *Fix an* $n \times (n-k)$ *matrix* Z *satisfying*

$$Y^t Z = 0 \quad \textit{and} \quad \text{rank}(Z) = n - k.$$

Then the following conditions are equivalent:

(1) $HY = YA$ *holds for some* $A : k \times k$.
(2) H *is of the form* $H = YKY^t + ZLZ^t$ *for some* $K \in \Omega_k$ *and some* $L \in \Omega_{n-k}$.

Now a necessary condition for an EDM to have $\mathbf{s}$-block structure is derived. Define the subvectors $\mathbf{s}_1, \ldots, \mathbf{s}_k$ of $\mathbf{s}$ as in Section 1, and suppose that the vectors $\mathbf{s}_1, \ldots, \mathbf{s}_k$ do not contain zero components, which implies that the matrix S in (1.4) is non-singular.

Theorem 3. *Suppose that* $D \in \Lambda_n$ *has* $\mathbf{s}$*-block structure for a vector* $\mathbf{s}$ *with no zero components. Then there exists a positive semidefinite matrix* $B = (b_{ij}) \in \Omega_n(\mathbf{s})$ *such that* $D = \kappa(B)$ *and*

$$B = \overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^t S^{-1} \quad \textit{for some } K \in \Omega_k(\boldsymbol{v}) \quad \textit{and} \quad L \in \Omega_{n-k}, \tag{2.3}$$

where $\boldsymbol{v} = (n_1, n_2, \ldots, n_k)^t \in \Re^k$. *Furthermore, the vector* $\mathbf{b} = (b_{11}, b_{22}, \ldots, b_{nn})^t \in \Re^n$ *is blocked*.

Proof. By assumption, D is an EDM satisfying

$$D\overline{S} = \overline{E}A \quad \text{for some } A : n \times k, \tag{2.4}$$

from which it follows that

$$D\overline{S}\boldsymbol{\epsilon} = \overline{E}A\boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \in \Re^k.$$

We can see that the above equality is equivalent to $D\mathbf{x} = \overline{E}\mathbf{v}$ by letting $\mathbf{x} = \overline{S}\boldsymbol{\epsilon}/n$ and $\mathbf{v} = A\boldsymbol{\epsilon}/n$. Hence the condition (a) of Theorem 1 is satisfied, and the vector $\mathbf{b}$ is blocked.

Choose $B \in \Omega_n(\mathbf{s})$ such that $D = \kappa(B)$. Then the equality (2.4) can be rewritten as

$$(\mathbf{e}\mathbf{b}^t + \mathbf{b}\mathbf{e}^t - 2B)\overline{S} = \overline{E}A. \tag{2.5}$$

Since the vector $\mathbf{b}$ is blocked, it can be written as

$$\mathbf{b} = \begin{pmatrix} \beta_1\mathbf{e}_1 \\ \beta_2\mathbf{e}_2 \\ \vdots \\ \beta_k\mathbf{e}_k \end{pmatrix} = \overline{E}\boldsymbol{\beta} \quad \text{for some} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} \in \Re^k. \tag{2.6}$$

Similarly, the vector $\mathbf{e}$ can be rewritten as

$$\mathbf{e} = \overline{E}\boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \in \Re^k. \tag{2.7}$$

By substituting (2.6) and (2.7) into (2.5), we can restate (2.5) as

$$\overline{E}(\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t)\overline{E}^t\overline{S} - 2B\overline{S} = \overline{E}A,$$

which implies that

$$B\overline{S} = \overline{E}\mathbb{A},$$

where $\mathbb{A} = \{(\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t)\overline{E}^t\overline{S} - A\}/2$. Multiplying the above equality by $S^{1/2}$ and using the relation $\overline{S} = S\overline{E}$ (see (1.5)) yield

$$S^{1/2}BS\overline{E} = S^{1/2}\overline{E}\mathbb{A}.$$

By letting $H = S^{1/2}BS^{1/2}$ and $Y = S^{1/2}\overline{E}$, we have

$$HY = Y\mathbb{A}. \tag{2.8}$$

Since H is positive semidefinite, Lemma 1 applies and hence (2.8) can be rewritten as

$$H = YKY^t + ZLZ^t \text{ for some } K \in \Omega_k \quad \text{and} \quad L \in \Omega_{n-k}, \tag{2.9}$$

where Z is an $n \times (n-k)$ matrix satisfying $Z^tY = 0$ and rank$Z = n - k$. Since $Y = S^{1/2}\overline{E}$ and $\overline{F}^t\overline{E} = 0$ (see (2.2)), we can choose

$$Z = S^{-1/2}\overline{F}.$$

Hence the equality (2.9) is expressed in the original notation as

$$B = \overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^tS^{-1} \quad \text{with } K \in \Omega_k \quad \text{and} \quad L \in \Omega_{n-k}.$$

It remains to show that $K \in \Omega_k(\boldsymbol{v})$. Since the matrix B is in $\Omega_n(\mathbf{s})$, it satisfies

$$0 = B\mathbf{s}.$$

Hence we have

$$\begin{aligned}0 &= \left[\overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^tS^{-1}\right]\mathbf{s}\\ &= \left[\overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^tS^{-1}\right]S\overline{E}\boldsymbol{\epsilon} \quad (\text{since } \mathbf{s} = S\overline{E}\boldsymbol{\epsilon})\\ &= \overline{E}K\overline{E}^tS\overline{E}\boldsymbol{\epsilon} \quad (\text{since } \overline{F}^t\overline{E} = 0)\\ &= \overline{E}K\boldsymbol{v} \quad (\text{since } \overline{E}^tS\overline{E}\boldsymbol{\epsilon} = \boldsymbol{v}),\end{aligned}$$

which implies $K\boldsymbol{v} = 0$ since $\overline{E}$ is of full rank. Thus $K \in \Omega_k(\boldsymbol{v})$ is obtained. □

The next theorem derives a sufficient condition for $D = \kappa(B)$ to have **s**-block structure. Since the vector **b** is assumed to be blocked, the theorem is slightly different from the converse of Theorem 3.

Theorem 4. *Suppose that $B \in \Omega_n(\mathbf{s})$ is of the form*

$$B = \overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^tS^{-1} \quad \text{for some } K \in \Omega_k(\boldsymbol{v}) \quad \text{and} \quad L \in \Omega_{n-k}, \tag{2.10}$$

*where $\boldsymbol{v} = (n_1, n_2, \ldots, n_k)$. If **b** is a block vector, that is, **b** can be written as*

$$\mathbf{b} = \overline{E}\boldsymbol{\beta} \quad \text{for some } \boldsymbol{\beta} \in \Re^k,$$

*then $D = \kappa(B)$ is an EDM having **s**-block structure. More specifically,*

$$D\overline{S} = \overline{E}A \quad \text{with } A = (\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t - 2K)\overline{E}^tS\overline{E}. \tag{2.11}$$

Proof. Clearly $D = \kappa(B)$ is an EDM. The matrix B satisfies

$$\begin{aligned}B\overline{S} &= \left[\overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^tS^{-1}\right]S\overline{E}\\ &= \overline{E}K\overline{E}^tS\overline{E} \quad (\text{since } \overline{F}^t\overline{E} = 0).\end{aligned} \tag{2.12}$$

Hence we have

$$\begin{aligned}D\overline{S} &= \kappa(B)\overline{S}\\ &= [\mathbf{e}\mathbf{b}^t + \mathbf{b}\mathbf{e}^t - 2B]\overline{S}\\ &= \mathbf{e}\mathbf{b}^t\overline{S} + \mathbf{b}\mathbf{e}^t - 2\overline{E}K\overline{E}^tS\overline{E},\end{aligned} \tag{2.13}$$

where (2.12) is used. Since $\mathbf{b} = \overline{E}\boldsymbol{\beta}$ and $\mathbf{e} = \overline{E}\boldsymbol{\epsilon}$ hold, the equality (2.13) is further rewritten as

$$\begin{aligned}DS\overline{E} &= \overline{E}\boldsymbol{\epsilon}\boldsymbol{\beta}^t\overline{E}^tS\overline{E} + \overline{E}\boldsymbol{\beta}\boldsymbol{\epsilon}^t\overline{E}^tS\overline{E} - 2\overline{E}K\overline{E}^tS\overline{E}\\ &= \overline{E}(\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t - 2K)\overline{E}^tS\overline{E}.\end{aligned}$$

Since $\overline{S} = S\overline{E}$, this completes the proof. □

The condition (1.8) is closely related to (2.11), since (1.8) can be rewritten as

$$A = (\boldsymbol{\epsilon}\mathbf{x}^t + \mathbf{x}\boldsymbol{\epsilon}^t)\overline{E}^tS\overline{E} \quad \text{for some } \mathbf{x} \in \Re^k.$$

3. Examples

Now we show a couple of examples that illustrate the decomposition of the matrix B in the previous theorems.

Example 1. Consider the case in which $L = 0$ in (2.10) in Theorem 4. That is, let $K = (x_{ij})$ be a $k \times k$ matrix such that $K \in \Omega_k(\boldsymbol{v})$, and let

$$B = \overline{E}K\overline{E}^t.$$

Then $B = (b_{ij}) \in \Omega_n(\mathbf{s})$. The (i,j)th block of B is given by

$$B_{ij} = x_{ij}\mathbf{e}_i\mathbf{e}_j^t \quad (i,j = 1,\ldots,k).$$

In this example, we show that the EDM $D = \kappa(B)$ has $\mathbf{s}$-block structure. Since the vector $\mathbf{b} = (b_{11}, \ldots, b_{nn})^t$ is calculated as

$$\mathbf{b} = \begin{pmatrix} x_{11}\mathbf{e}_1 \\ \vdots \\ x_{kk}\mathbf{e}_k \end{pmatrix} = \overline{E}\boldsymbol{\beta} \quad \text{with } \boldsymbol{\beta} = \begin{pmatrix} x_{11} \\ \vdots \\ x_{kk} \end{pmatrix},$$

the EDM $D = \kappa(B)$ is obtained as

$$D = (D_{ij}) \quad \text{with } D_{ij} = (x_{ii} + x_{jj} - 2x_{ij})\mathbf{e}_i\mathbf{e}_j^t : n_i \times n_j.$$

Then the direct calculation shows that

$$D_{ij}\mathbf{s}_j = (x_{ii} + x_{jj} - 2x_{ij})n_j\mathbf{e}_i \quad (i,j = 1,\ldots,k),$$

or equivalently,

$$D\overline{S} = \overline{E}A \quad \text{with } A = (\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t - 2K)\overline{E}^t S\overline{E}.$$

Hence D is an EDM having $\mathbf{s}$-block structure. $\square$

By using the following lemma, we can construct an example of B in (2.3) such that $\mathbf{b}$ is a block vector.

Lemma 2. *Let H and Z be $m \times m$ diagonal matrices*

$$H = \begin{pmatrix} h_1 & & 0 \\ & \ddots & \\ 0 & & h_m \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} w_1 & & 0 \\ & \ddots & \\ 0 & & w_m \end{pmatrix},$$

where $h_1, \ldots, h_m \neq 0$ and hence H is non-singular. Let

$$M = I_m - (1/m)\mathbf{e}\mathbf{e}^t, \quad \mathbf{h}^2 = (h_1^2, \ldots, h_m^2)^t, \quad \mathbf{w} = (w_1, \ldots, w_m)^t.$$

Then the following two statements are equivalent:

(a) *The following equality holds for some $c > 0$:*

$$\mathbf{w} = \frac{cn}{n-2}\left[I_m - \frac{1}{m(m-1)}\mathbf{e}\mathbf{e}^t\right]\mathbf{h}^2; \tag{3.14}$$

(b) *All the diagonal elements of $H^{-1}MWMH^{-1}$ are equal to c.*

Proof. First we derive a condition for these diagonal elements to be equal to 1. Next we move on to the general case.

Since the ith diagonal element of $H^{-1}MWMH^{-1}$ is given by

$$\left\{ w_i - 2w_i/m + (1/m^2)\sum_{j=1}^{m} w_j \right\} \Big/ h_i^2, \tag{3.15}$$

all the diagonal elements are equal to 1 if and only if

$$\left\{ w_i - 2w_i/m + (1/m^2)\sum_{j=1}^{m} w_j \right\} = h_i^2 \quad (i = 1,\ldots,m),$$

which can be rewritten as

$$\left[\left(1-\frac{2}{m}\right)I_n+\frac{1}{m^2}\mathbf{e}\mathbf{e}^t\right]\mathbf{w}=\mathbf{h}^2.$$

Since

$$\left[\left(1-\frac{2}{m}\right)I_m+\frac{1}{m^2}\mathbf{e}\mathbf{e}^t\right]^{-1}=\frac{m}{m-2}\left[I_m-\frac{1}{m(m-1)}\mathbf{e}\mathbf{e}^t\right],$$

we have

$$\mathbf{w}=\frac{m}{m-2}\left[I_m-\frac{1}{m(m-1)}\mathbf{e}\mathbf{e}^t\right]\mathbf{h}^2. \tag{3.16}$$

Hence we can see that the diagonal elements of $H^{-1}MWMH^{-1}$ are equal to 1 if and only if the diagonal elements of W are given by $\mathbf{w}$ in (3.16). From this, it readily follows that the diagonal elements of $H^{-1}MWMH^{-1}$ are identical to $c>0$ if and only if the diagonal elements of W are given by $\mathbf{w}$ in (3.14). $\square$

Example 2. Next we consider the case where K and L in (2.10) are of simple structure. More precisely, let $K=0$ and let B be of the form

$$B=S^{-1}\overline{F}L\overline{F}^tS^{-1}\quad\text{with}\ L=\overline{F}^tW\overline{F}, \tag{3.17}$$

where W is an $n\times n$ diagonal matrix. Decompose W according to S as

$$W=\begin{pmatrix}W_1 & & 0\\ & \ddots & \\ 0 & & W_k\end{pmatrix},\quad S=\begin{pmatrix}S_1 & & 0\\ & \ddots & \\ 0 & & S_k\end{pmatrix}\quad\text{with}\ W_i,S_i:n_i\times n_i.$$

Then the matrix L is written as the following block diagonal matrix:

$$L=\begin{pmatrix}F_1^tW_1F_1 & & 0\\ & \ddots & \\ 0 & & F_k^tW_kF_k\end{pmatrix}.$$

Hence the matrix B is also a block diagonal matrix:

$$B=\begin{pmatrix}S_1^{-1}F_1F_1^tW_1F_1F_1^tS_1^{-1} & & 0\\ & \ddots & \\ 0 & & S_k^{-1}F_kF_k^tW_kF_kF_k^tS_k^{-1}\end{pmatrix}.$$

Since $F_iF_i^t=I_{n_i}-(1/n_i)\mathbf{e}_i\mathbf{e}_i^t=M_i$ (say), each diagonal block B_{ii} of B is of the form

$$B_{ii}=S_i^{-1}F_iF_i^tW_iF_iF_i^tS_i^{-1}=S_i^{-1}M_iW_iM_iS_i^{-1},$$

and hence we can apply Lemma 2 to B_{ii}. For each i, let $\mathbf{w}_i$ and $\mathbf{s}_i^2$ be the $n_i\times 1$ vectors that consist of the diagonal elements of W_i and S_i, respectively. Suppose that $\mathbf{w}_i$ and $\mathbf{s}_i^2$ satisfy

$$\mathbf{w}_i=\frac{c_in_i}{n_i-2}\left[I_{n_i}-\frac{1}{n_i(n_i-1)}\mathbf{e}_i\mathbf{e}_i^t\right]\mathbf{s}_i^2\quad\text{for some}\ c_i>0\quad(i=1,\dots,k).$$

Then, by Lemma 2, each B_{ii} has equal diagonal elements c_i. Thus we see that the vector $\mathbf{b}=(b_{11},\dots,b_{nn})^t$ is a block vector:

$$\mathbf{b}=\begin{pmatrix}c_1\mathbf{e}_1\\ \vdots\\ c_k\mathbf{e}_k\end{pmatrix}=\overline{E}\boldsymbol{\beta}\quad\text{with}\ \boldsymbol{\beta}=\begin{pmatrix}c_1\\ \vdots\\ c_k\end{pmatrix}.$$

Hence by Theorem 4, the EDM $D = \kappa(B)$ has **s**-block structure: More specifically, we can see

$$D\overline{S} = \overline{E}A \quad \text{with } A = (\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t)\overline{E}^t S\overline{E}. \quad \square$$

Now we will provide our last example for this section.

Example 3. A more general case can be easily obtained by combining the above two examples. Let L be the matrix given in Example 2 and let $K = (x_{ij})$ be any matrix in $\Omega_k(\boldsymbol{v})$. Then from Examples 1 and 2, the matrix B given below

$$B = \overline{E}K\overline{E}^t + S^{-1}\overline{F}L\overline{F}^t S^{-1}$$

satisfies the condition of Theorem 4. Hence the EDM $D = \kappa(B)$ has **s**-block structure. In fact, it readily follows from Examples 1 and 2 that

$$\mathbf{b} = \begin{pmatrix} (x_{11} + c_1)\mathbf{e}_1 \\ \vdots \\ (x_{kk} + c_k)\mathbf{e}_k \end{pmatrix} = \overline{E}\boldsymbol{\beta} \quad \text{with } \boldsymbol{\beta} = \begin{pmatrix} x_{11} + c_1 \\ \vdots \\ x_{kk} + c_k \end{pmatrix},$$

which implies that

$$D\overline{S} = \overline{E}A \quad \text{with } A = (\boldsymbol{\epsilon}\boldsymbol{\beta}^t + \boldsymbol{\beta}\boldsymbol{\epsilon}^t - K)\overline{E}^t S\overline{E}.$$

3.1. A numerical example

At this point a numerical example will show the reason of the decomposition of the matrix B, which implies a decomposition of the matrix $D = \kappa(B)$ since the application κ is linear.

We will build the configuration by pieces to show how the decomposition appears. The values are standard Matlab outputs. We will generate a configuration in $\Re^2$ by defining the following matrices:

$$X_1 = \begin{pmatrix} 0.8000 & 0.6000 \\ -0.8000 & 0.6000 \\ 0 & -1.0000 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0.4000 & 1.9596 \\ 0.4000 & -1.9596 \\ -2.0000 & 0 \end{pmatrix},$$
$$X_3 = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}.$$

Now we imbed them in the three dimensional space as follows:

$$\widehat{X}_1 = \begin{pmatrix} 0.8000 & 0.6000 & 1 \\ -0.8000 & 0.6000 & 1 \\ 0 & -1.0000 & 1 \end{pmatrix}, \quad \widehat{X}_2 = \begin{pmatrix} 0.4000 & 1.9596 & 2 \\ 0.4000 & -1.9596 & 2 \\ -2.0000 & 0 & 2 \end{pmatrix},$$
$$\widehat{X}_3 = \begin{pmatrix} 1 & 1 & -3 \\ -1 & -1 & -3 \end{pmatrix}.$$

These last three configurations are translations of the previous ones along the "z" axis.

Now we form the coordinate matrix X

$$X = \begin{pmatrix} 0.8000 & 0.6000 \\ -0.8000 & 0.6000 \\ 0 & -1.0000 \\ 0.4000 & 1.9596 \\ 0.4000 & -1.9596 \\ -2.0000 & 0 \\ 1 & 1 \\ -1 & -1 \end{pmatrix},$$

which satisfy the condition (b) of Theorem 2.

We also form the corresponding matrix for the configurations in the three dimensional space.

$$\widehat{X} = \begin{pmatrix} 0.8000 & 0.6000 & 1 \\ -0.8000 & 0.6000 & 1 \\ 0 & -1.0000 & 1 \\ 0.4000 & 1.9596 & 2 \\ 0.4000 & -1.9596 & 2 \\ -2.0000 & 0 & 2 \\ 1 & 1 & -3 \\ -1 & -1 & -3 \end{pmatrix}.$$

The vector $\mathbf{s}$ for the configuration X is

$$\mathbf{s} = (\mathbf{s}_1^t, \mathbf{s}_2^t, \mathbf{s}_3^t)^t = (0.3125, 0.3125, 0.3750; 0.4167, 0.4167, 0.1667; 0.5000, 0.5000)^t,$$

where $\mathbf{s}_1$ is the vector with the first three components of $\mathbf{s}$ and $\mathbf{s}_2$ the following three components and $\mathbf{s}_3$ the last two. This vector also works for $\widehat{X}$.

But $\widehat{X}$ does not satisfy the condition (b) of Theorem 2. In fact, for example, $\widehat{X}_1\mathbf{s}_1$ is not zero. Hence $\widehat{X}$ does not have the origin representation property.

If we define by $\widehat{X}_{12}$ the matrix that has the first two columns of $\widehat{X}$ and by $\widehat{X}_3$ the matrix that has the third column of $\widehat{X}$, then

$$\widehat{X}\widehat{X}^t = \widehat{X}_3\widehat{X}_3^t + \widehat{X}_{12}\widehat{X}_{12}^t.$$

Now it is clear that the first term correspond to the first term in in the decomposition of Theorem 2.3 and the second term to the second.

Note that in Theorem 2.3, the first term is a block matrix, that in this example is coming from the coordinate of the centers of the spheres in the planes $z = 1$, $z = 2$ and $z = -3$. They are not anymore the origin of coordinates.

In other words, this work as if you think of every spherical configuration with all the points in the center of that sphere, this way you have repeated points that give you the block structure.

Following the theoretical description, the X matrix in Theorem 2.3 is $X = WW^t$ for

$$W = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 2 \\ 0 & 0 & -3 \end{pmatrix}.$$

The decomposition split the structure of the configuration in two. One corresponds to the centers of each subconfiguration and the rest to the structure of all the subconfigurations in a common embedding dimension.

It is clear that in this example we located the centers in a one dimensional configuration, but is possible to locate the center in any allowed dimension.

4. Multispherical structure and faces

In this section we consider how the multispherical structure of a configuration provides information about the location of the corresponding distance matrix in the cone of Euclidean distance matrices. For those matrices that are always located in the boundary of Λ_n, we can determine a number of supporting hyperplanes that are associated with the multispherical structure of the matrix.

We will start with a set of n points whose coordinates are the rows of the coordinate matrix X. The matrix D will denote the corresponding distance matrix: $D = \kappa(XX^t)$.

A multispherical configuration with k spheres, generates a partition of the set $\mathcal{N} = \{1, \ldots, n\}$ with k subsets $\mathcal{N}_j$. Each of these subsets contain the indexes corresponding to the points in each sphere. We denote their cardinality by n_j for $j = 1, \ldots, k$.

We also assume here that the points in each sphere can generate the origin of the system of coordinates. Technically this means that there are k vectors $\mathbf{s}_j \in \Re^{n_j}$ which satisfy

$$X_{\mathcal{N}_j}^t \mathbf{s}_j = 0$$

with $\mathbf{e}_j^t\mathbf{s}_j = 1$, where $\mathbf{e}_j$ is defined in (1.2). If we define $\mathbf{s}^t = (\mathbf{s}_1^t, \ldots, \mathbf{s}_k^t)$, we have that $\mathbf{s}^t\mathbf{e} = k$, and $\frac{1}{k}\mathbf{s} = 1$ is a system of coordinates, where $\mathbf{e} = (\mathbf{e}_1^t, \ldots, \mathbf{e}_k^t)^t$. We will refer to this property as origin multiple representation. In other words the origin of coordinates is a linear combination of the points in each sphere.

We can define now the vector $\bar{\mathbf{s}}_j \in \Re^n, j = 1, \ldots, k$ as follows:

$$(\bar{\mathbf{s}}_j)_{\mathcal{N}_m} = \begin{cases} \mathbf{s}_j & \text{if } m = j, \\ 0 & \text{otherwise.} \end{cases}$$

It is clear that $\bar{\mathbf{s}}_j, j = 1, \ldots, k$ belong to the null space of X^t, and $\bar{\mathbf{s}}_j^t\mathbf{e} = 1$, then they are systems of coordinates. Note by the way that these vectors are orthogonal, $\mathbf{s} = \sum_{i=1}^k \bar{\mathbf{s}}_j$ and s is in the $N(\tau_s(D))$.

From [6] we know that $LGS(D) = N(D) \oplus \langle \mathbf{x} \rangle$ where $\mathbf{x}$ solves the system $D\mathbf{x} = \mathbf{e}$. Remember that $LGS(D) \subset M$ and then it is orthogonal to $\mathbf{e}$. Hence we need look for vectors in $N(\tau_s(D))$ that are orthogonal to e.

Let us define vectors $\mathbf{u}_i$ for $i = 1, \ldots, k-1$ as $\mathbf{u}_i = \bar{\mathbf{s}}_i - \alpha_i\bar{\mathbf{s}}_k$, where α_i is determined in such a way that the vectors $\mathbf{u}_i$ for $i = 1, \ldots, k-1$ are orthogonal to $\mathbf{e}$. In other words

$$\mathbf{e}^t\mathbf{u}_i = \mathbf{e}^t(\bar{\mathbf{s}}_i - \alpha_i\bar{\mathbf{s}}_k) = \mathbf{e}^t\bar{\mathbf{s}}_i - \alpha_i\mathbf{e}^t\bar{\mathbf{s}}_k = 0.$$

Then

$$\mathbf{u}_i = \bar{\mathbf{s}}_i - \frac{\mathbf{e}^t\bar{\mathbf{s}}_i}{\mathbf{e}^t\mathbf{s}_k}\bar{\mathbf{s}}_k.$$

For our next result we need to use the Frobenius inner product in the space of matrices that is defined by $\langle A, B\rangle_F = trace(A^tB)$.

Theorem 5. *The vectors*

$$\mathbf{u}_i = \bar{\mathbf{s}}_i - \frac{\mathbf{e}^t\bar{\mathbf{s}}_i}{\mathbf{e}^t\mathbf{s}_k}\bar{\mathbf{s}}_k.$$

belong to $LGS(D)$ *and the hyperplanes*

$$\langle Z, \mathbf{u}_i\mathbf{u}_i^t\rangle_F = 0 \quad \textit{for } i = 1, \ldots, k-1$$

are supporting hyperplanes for D.

Proof. It is clear from construction that the vector $\mathbf{u}_i, i = 1, \ldots, k-1$ are orthogonal to the vector $\mathbf{e}$, and included in $N(\tau_s(D))$. Using Lemma 2 in [6] (see the proof) if we show that the vectors $\mathbf{u}_i, i = 1, \ldots, k-1$ are in $N(\tau_e(D))$, then they are in $LGD(D)$.

Using [3], it is easy to see that $B_e = \left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right) B_s \left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right)$ then computing $B_e\mathbf{u}_i$, we obtain

$$\left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right) B_s \left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right) \mathbf{u}_i = \left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right) B_s \left(\mathbf{u}_i - \frac{\mathbf{e}^t\mathbf{u}_i}{n}\mathbf{e}\right) = \left(I - \frac{\mathbf{e}\mathbf{e}^t}{n}\right) B_s\mathbf{u}_i = 0.$$

The second part of the theorem is a consequence of the fact that the vectors $\mathbf{u}_i$ belong to the $LGS(D)$. See [6] for details. □

Remark. It is important to point out that these vectors $\mathbf{u}_i, i = 1, \ldots, k-1$, which are linear combinations of the vectors $\bar{\mathbf{s}}_i$, are connected with the multispherical structure, better than that to the origin multiple representation property. Perturbations in D that preserve the origin multiple representation property will keep these vector associated with the perturbed matrix.

Let us consider a class of perturbations of the coordinate matrix X and of course the corresponding matrix D. Consider a positive constant block vector $\mathbf{w} = (w_1, \ldots, w_n)^t \in \Re^n$ respect to the partition $\mathcal{N}$ given above. This says that $w_i = \omega_j$ for $i \in \mathcal{N}_j$, where the vector $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_k)^t \in \Re^k$. We denote by W the diagonal matrix whose diagonal entries are given by the vector $\mathbf{w}$. Then we consider the family of coordinate matrices $X_w = WX$, and distance matrices D_w where $D_w = \kappa(X_wX_w^t)$.

Corollary 1. *The hyperplanes*

$$\langle Z, \mathbf{u}_i\mathbf{u}_i^t\rangle_F = 0 \quad \textit{for } i = 1, \ldots, k-1$$

are supporting hyperplanes for any matrix in the family D_W.

Proof. This is the result of the following simple computation:

$$X_W^t\bar{\mathbf{s}}_j = X_{\mathcal{N}_j}\omega_j\mathbf{s}_j = \omega_j X_{\mathcal{N}_j}\mathbf{s}_j = 0,$$

which means that the vector $\mathbf{u}_i$, $i = 1, \ldots, k-1$ are also in the null space of $B_W = X_W X_W^t$. □

We emphasize here that all the member of the family are in the face determined by the intersection of the supporting hyperplanes.

Also it is worthy to note that if $r_j, j = 1, \ldots, k$ are the radii of the spheres of the multispherical configuration, then the configuration WX with $\omega_j = \frac{1}{r_j}, j = 1, \ldots, k$ is spherical. This fact point out the importance of the partition with the origin multiple representations property in the generation of multispherical configurations.

Finally, we show that this multispherical structure allows us to built vector in the null space of D. Since this relays in the vectors $\tilde{\mathbf{s}}_j' j = 1, \ldots, k$ and $\mathbf{u}_j, j = 1, \ldots, k-1$ the result are true for the family D_W.

To simplify the notation let us denote by $\widehat{B}$ the matrix $\tau(D)$ and by $\hat{\mathbf{b}}$ the vector that contain the diagonal entries of $\widehat{B}$. Now Let us define the vectors $\mathbf{y}_j, j = 1, \ldots k-2$ given by the following expression:

$$\mathbf{y}_j = \mathbf{u}_j - \frac{\hat{\mathbf{b}}^t\mathbf{u}_j}{\hat{\mathbf{b}}^t\mathbf{u}_{k-1}}\mathbf{u}_{k-1}, \quad j = 1, \ldots, k-2.$$

Note that this orthogonalization process can be avoided for the vectors $\mathbf{u}_j$ that are already orthogonal to $\hat{\mathbf{b}}$.

Theorem 6. *The vectors* $\mathbf{y}_j, j = 1, \ldots k-2$ *are in* $N(D)$.

Proof. The following computation shows that the vectors $\mathbf{y}_j$ are in $N(D)$:

$$D\mathbf{y}_j = (\mathbf{e}\mathbf{b}^t + \mathbf{b}\mathbf{e}^t - 2\widehat{B})\mathbf{y}_j = (\mathbf{b}^t\mathbf{y}_j)\mathbf{e} + (\mathbf{e}^t\mathbf{y}_j)\mathbf{b} - 2\widehat{B}\mathbf{y}_j$$

since the vectors $\mathbf{y}_j$ are orthogonal to $\mathbf{e}$ because they are linear combination of the vectors $\mathbf{u}_i$ and orthogonal to $\hat{\mathbf{b}}$ for construction. Note also that the vectors $\mathbf{y}_j$ are in the null space of $\widehat{B}$. □

It is straightforward that the vectors $\mathbf{y}_i, i = 1, \ldots, k-2$ are combination of three of the $\bar{\mathbf{s}}_j, j = 1, \ldots, k$, which means that a good part of the structure of D_W is coming from the multispherical structure with the multiple origin representation property.

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